

DETAILED COMPUTATIONAL MODELING OF MILITARY INCINERATORS

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ABSTRACT

The United States has selected incineration as one of the methods for destroying the highly toxic chemical agents and munitions contained within the Chemical Weapons Stockpile. In this paper we describe a suite of Computational Fluid Dynamic (CFD) based models that provide the ability to conduct detailed simulations of chemical demilitarization incinerator operation. The models contain 3D furnace and canister geometries and all of the relevant physics and chemistry. The destruction of chemical agent is predicted using non-equilibrium chemistry models that include full and reduced chemical kinetic mechanisms. We have developed CFD models for a Liquid Incinerator, Metal Parts Furnace, Metal Parts Furnace Afterburner, and a De-Activation Furnace System located at the Tooele Chemical Agent Disposal Facility (TOCDF), in Tooele, Utah. We modeled the incineration of the GB agent using the simulant dimethyl methylphosphonate (DMMP). The models predict complete destruction of the chemical agent when the incinerators and afterburners are operated as per standard operating conditions.

NOTATION

CARM	Computer Automated Reduction Method
CFD	Computational Fluid Dynamics
CSDP	Chemical Stockpile Disposal Program
DFS	Deactivation Furnace System
DMMP	dimethyl methylphosphonate
GB	Sarin
LIC	Liquid Incinerator Furnace
MPF	Metal Parts Furnace
PFR	Plug flow reactor
REI	Reaction Engineering International
TOCDF	Tooele Chemical Agent Disposal Facility
T ₉₉	Temperature requirement for 99% destruction
VX	VX nerve gas

INTRODUCTION

The U.S. stockpile of chemical weapons consist of munitions, including mines, rockets, artillery shells, and bombs containing warfare agents stored at eight sites in the continental United States and on Johnston Island in the Pacific Ocean. The chemical warfare agents (CWA) consist of mustard gas, blister agents, and organo-phosphorus nerve agents. Incineration has been used to destroy the stockpiles at Johnston Island, is currently being used to destroy the

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stockpile at Toole in Utah, and incinerators are under construction at three sites (Anniston Army Depot, Anniston, AL; Pine Bluff Arsenal, Pine Bluff, AK; and Umatilla Depot, Umatilla, OR

In this paper we describe component models for a selected subset of the incinerators and afterburners at the Tooele Chemical Agent Disposal facility (TOCDF). We chose to use the incinerators at the TOCDF because the incinerators to be used at other Army incineration sites will use systems similar (some are identical) to those at the TOCDF. These models are to help with: (1) assessing the health and environmental impact of the incinerators, (2) evaluating potential opportunities to enhance online availability and to increase munitions throughput, and (3) assessing problems with decommissioning and retroactive assessments of questions that may arise after closure.

The three incineration systems and their associated afterburners modeled in this paper are:

- The Liquid Incinerator Furnace (LIC) used to incinerate the liquid CWA drained from the munitions;
- The Metals Parts Furnace (MPF) designed to decontaminate the drained shells, and
- The Deactivation Furnace (DFS) used to deactivate the energetic materials used as propellants and fuses in the munitions.

In this paper we only model the destruction of a surrogate for GB agent. The chemistry for the destruction of the surrogate is described first and then it is incorporated into CFD models of the LIC, MPF, and DFS.

PYROLYSIS AND FLAME CHEMISTRY

Chemistry of Agent Destruction

The models are configured to simulate the thermal destruction of the nerve agent GB (Sarin). Lacking a chemical mechanism for the thermal destruction of GB, we used as a surrogate dimethyl methylphosphonate (DMMP), a compound that is chemically similar to GB. The DMMP mechanism used in this study is based on the mechanism of Werner and Cool [1], with modifications by Wainner et al. [2]. This mechanism contains 63 species and 436 reactions. In addition to pyrolytic decomposition, this mechanism accounts for the H and OH radical attack mechanisms that dominated under the low temperature ($T < 1500$ K), fuel-rich H_2 - O_2 flame conditions studied by Werner & Cool [1], as well as attack by O and methyl radicals encountered in significant concentrations in the fuel-lean hydrocarbon flames used in incineration equipment.

Calculations with the DMMP mechanism show DMMP to be thermally unstable. Even in the absence of other reactants, DMMP is easily destroyed. In these calculations the DMMP was mixed with nitrogen so the initial destruction is due entirely to unimolecular decomposition. When DMMP is added to equilibrated rich methane air combustion products destruction occurs at lower temperatures. Agents are relatively unstable, ranking low on the hazardous organic compound incinerability index. For example, mustard agent ranked 132, just below 1,1 dichloroethane [3]. This can be compared with HCN that ranked first and benzene second on this index. The temperature requirement for 99 percent destruction (T_{99}) for HCN and benzene are $>1150^\circ\text{C}$ and $\sim 1150^\circ\text{C}$, respectively. By contrast mustard gas has a T_{99} of less than 680°C [3]. Our calculations of T_{99} for DMMP give a value of 900°C .

Integration of Detailed Chemistry Along Streamlines

A tool has been developed that allows information to be extracted from CFD simulation results giving information about the flow and reactions along a streamline. Given a starting location, this tool will tabulate the temperature, species concentrations, velocities, or any other quantity from the CFD simulation as a function of time along the path that would be experienced by an infinitesimal fluid element. This time and species history information can be input to a modified version of the SENKIN code that calculates detailed chemical kinetics in a plug flow reactor (PFR). Thus, both temperature and major species (N_2 , H_2 , H_2O , CO , CO_2 , O_2) concentrations can be interpolated from a CFD simulation along a streamline and specified as functions of time within the PFR calculation. This allows detailed chemical kinetics to be used for post-processing a CFD simulation, while incorporating effects of mixing and heat release from the CFD simulation. In all cases we demonstrated very rapid and complete destruction of the agent simulant. However, this streamline approach extracts only mean information from the CFD solution and thus neglects turbulent fluctuations. Consequently it is important that a reduced mechanism that replicates the results

of the full mechanism over the conditions of interest is available and can be added to the CFD modules to account for the interaction of chemistry and turbulence.

Applicability of Reduced Mechanisms

Reduced mechanisms for DMMP combustion with 15 and 21 species have been created using the automatic mechanism reduction software CARM [5]. Both reduced mechanisms compare well to the full mechanism in simple reactor test cases. The smaller reduced mechanism has been implemented into the CFD post processing software.

The CARM software is able to create reduced mechanisms from the detailed mechanisms. The first step in this process is to create a “skeletal mechanism” by using sensitivity analysis to remove species and reaction steps that are unimportant at the conditions of interest. This resulted in a skeletal mechanism with 47 of the original 63 species and 149 of the original 436 reactions. From this skeletal mechanism, reduced mechanisms containing 15 and 21 species were created. Comparisons between full and reduced mechanisms were made of DMMP destruction in a fixed-temperature perfectly stirred reactor (PSR) for stoichiometric methane/air with 1000 ppm of DMMP added. Both reduced mechanisms gave reasonable results. These mechanisms were both optimized for conditions in the MPF afterburner, i.e. lean stoichiometry, $T = 1200\text{--}1800\text{ K}$. The reduced mechanisms cannot be expected to perform well outside this range of conditions. Reduced mechanisms can be created to model a broader range of conditions, but may require retaining more species.

The 15-species reduced mechanism includes the species N_2 , H_2 , O_2 , H_2O , H , O , OH , CH_4 , CH_3 , CO , CO_2 , PO_2 , HOPO_2 , $\text{OP}(\text{OH})_3$, and DMMP. This mechanism has been implemented into REI’s in-house CFD post-processing software. This code uses the temperature and velocity fields calculated using equilibrium chemistry as a background for calculations of chemical kinetic effects using the reduced mechanism. REI has previously successfully applied this technique to NO_x reduction by injection of ammonia and urea reagents in the upper part of a coal fired utility boiler [6]. The reduced mechanism post-processing code has been applied to the MPF afterburner base case and upset case with one burner disabled assuming extraordinarily poor performance of the MPF in which 1000 ppm of agent simulant enters the afterburner. Extremely high destruction efficiency is predicted in both cases.

INCINERATION CFD MODELS

Models have been constructed and tested for 1) the Liquid Incinerator (LIC); 2) the Metal Parts Furnace (MPF) primary chamber, 3) the MPF afterburner, and 4) the Deactivation Furnace System (DFS) rotary kiln. This section will present results for each of these models.

Incinerator-specific submodels such as a munitions/agent transient heat transfer model for the MPF and an energetics combustion model for the DFS kiln were developed as stand-alone computer programs, and are not coupled with the respective reacting CFD code.

CFD Modeling Approach for Incinerator Components

The technical approach used to produce the furnace module involved the following:

1. REI’s reacting two-phase CFD code, *GLACIER*, predicted the temperature and flow fields using equilibrium chemistry with an assumed shape probability density function (PDF) to account for turbulence chemistry interactions.
2. To reduce the required memory, only a subset of the species contained in the detailed mechanism was used in the CFD calculations involving equilibrium chemistry. These species included major reactant and product species with relatively few intermediates. The species subset was selected to reproduce the adiabatic flame temperature obtained with the complete list of the species in the mechanism over a wide range of stoichiometries.
3. Finite rate kinetic calculations either by the streamline approach or the reduced mechanism were then applied as a post-process using the previously calculated temperature and flow fields.

It is important to gauge the significance of flame suppression and understand under what conditions it occurs because the CFD models used in this project use an equilibrium chemistry approximation, which is unable to account for these effects. The approach we are adopting in developing incinerator models is to obtain the flow and temperature fields from CFD models assuming chemical equilibrium followed by detailed chemistry calculations as a post-

process. A study was performed to investigate the validity of equilibrium chemistry to obtain the overall heat release and resulting flow field. The study showed that the blowout residence time increases as more DMMP is added, demonstrating the well-known flame suppression characteristics of organo-phosphorus compounds. These studies suggest that inhibition only occurs at combustion intensities (very short residence times or high strain rates) much greater than are encountered in the incineration units.

The addition of phosphorus compounds to flames can also result in a significant increase in temperature due to the resulting enhancement of exothermic radical recombination reactions. Our calculations show that addition of up to a few thousand ppm of DMMP to a methane-air flame has a very small effect ($<5\text{K}$) on the equilibrium temperature, but can significantly increase the temperature (100-150 K) of an intermediate residence time (0.001 sec.) stirred reactor flame that lies between extinction and equilibrium conditions. Glaude et al. [7] reached similar conclusions from simulations of premixed flames to which DMMP was added. Twarowski [8] suggested adding phosphorus to rocket propellants to lessen dissociation losses and improve performance. Thus, for conditions under which extinction does not occur, the phosphorus compounds will speed the equilibration of the system, improving the validity of our CFD approach. These results suggest that organo-phosphorus flame suppression is not an important effect in the systems being modeled, justifying our modeling approach.

The Liquid Incinerator CFD Model

The liquid injection furnace is used to dispose of chemical agent drained from storage tanks and munitions. It uses an air atomized drained agent spray and an auxiliary fuel (natural gas) vortex burner firing into a refractory lined chamber. Figure 1a shows the temperature field in the horizontal vortex burner as it enters the vertical cylindrical LIC chamber. The LIC afterburner was not modeled.

It was necessary to model the vaporization of the GB simulant, DMMP. The vapor pressure data and gas thermodynamic data available for the simulant were used with the Clapeyron Equation to generate the thermodynamic data for the liquid phase. This was needed so that the existing model, which REI has previously used to model particle drying and water droplet vaporization, could be used for agent droplet vaporization. The droplet size distribution of the spray was determined from a correlation for air blast atomizers [9]. Conservation of momentum between the atomization air and liquid stream dictated the starting velocities of the droplets.

Figure 1a shows the predicted gas temperatures and droplet trajectories in the vortex chamber. Combustion is almost complete within the burner chamber. When the droplet trajectories terminate, the droplets have evaporated. At this point the agent has been completely released into the gas phase. The internal recirculation zone induced by the swirling air flow enhances the mixing resulting in chamber exit conditions that are well mixed with only a slight stratification in O_2 concentration. The exit O_2 was predicted at 5.4% wet (6.1% dry) consistent with complete combustion. The detailed DMMP chemistry was integrated along streamlines within the LIC for the streamlines shown in Fig. 1a. The results of these integrations are shown in Fig. 1b, showing the calculated DMMP mole fraction. This calculation assumes that pure agent (mole fraction = 1) exists at the beginning of each streamline. Temperature and major species (N_2 , H_2 , H_2O , CO , CO_2 , O_2) concentrations were interpolated from the CFD simulation along a streamline and specified as functions of time within the kinetics integration. The mole fraction associated with the detection limit is shown in red. The line in purple represents the level at which the last molecule of agent is destroyed. The initial number of molecules is that number that enters the furnace over the residence time of streamline 1 (0.7 sec). The location along the streamlines where the last molecule of agent has been destroyed is roughly at the position of maximum temperature within the flame, which is just outside the vortex chamber.

NO_x was also calculated for the baseline case of the LIC using REI's code, *GLACIER*. The model accounts for thermal, fuel and prompt NO_x formation as well as destruction under fuel rich conditions. Since there is no nitrogen in the agent or fuel, all of the NO_x is formed from molecular nitrogen in the air, that is, thermal NO_x . The regions of highest NO_x formation are coincident with regions of highest temperature. The predicted NO_x formation in the primary chamber is low (0.044 lb NO_x per MBtu).

One challenge at facility closure is how to dispose of potentially contaminated material. One such example is the carbon filter material that is in the air filtration system. One possibility is to grind the material and burn it either dry or as a slurry. We have simulated a case in which the fine carbon particles were injected pneumatically into the LIC. The flow rate of the carbon and liquid agent was adjusted to provide 5% of the heat input from the carbon. The natural gas flow rate was unchanged. The total heat input was the same as the baseline case. Carrier air was used to inject the carbon particles such that the particle loading of the injection stream was 0.5 lb particles per lb air. The

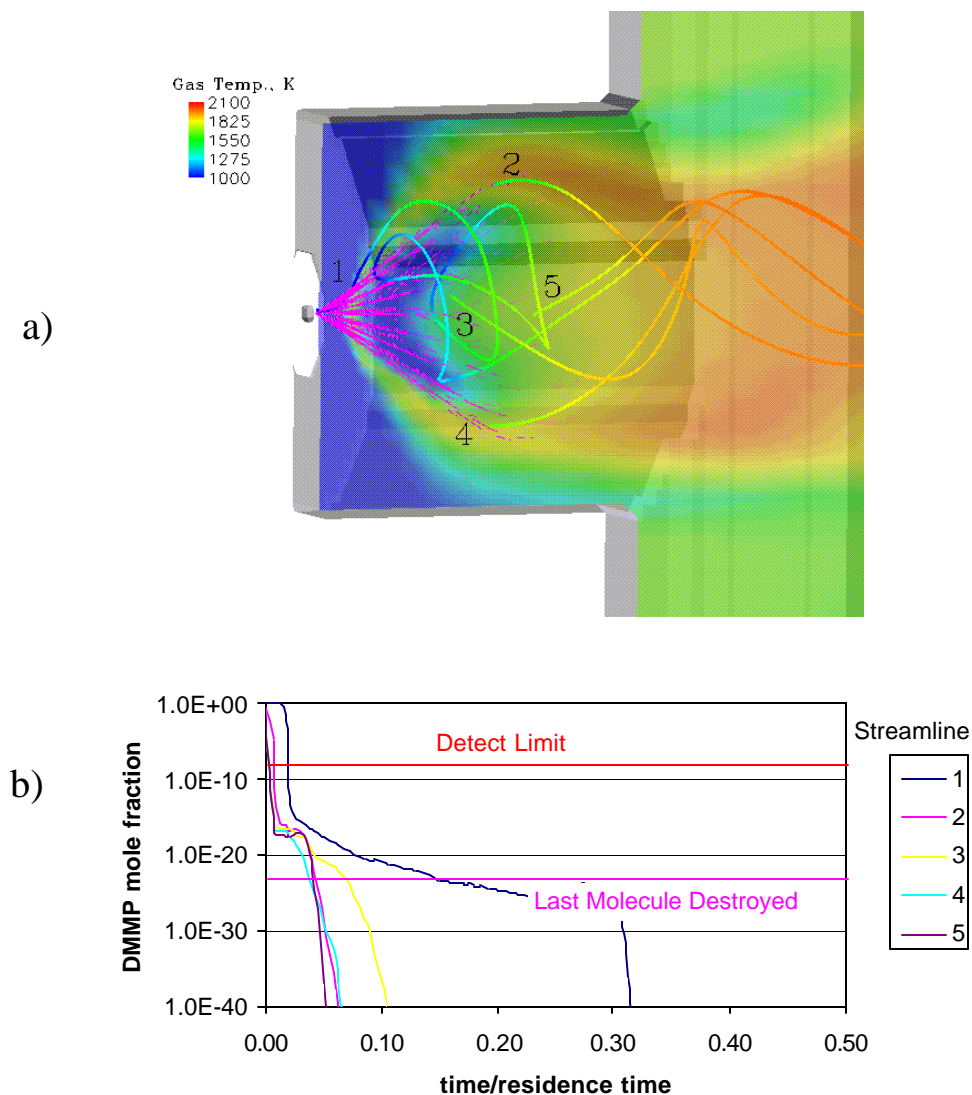


Figure 1 a) Predicted gas temperatures and droplet trajectories in the LIC vortex chamber. b) DMMP mole fraction calculated along streamlines from LIC primary chamber. (residence time = 0.7 sec.)

carbon particles were made up of three size fractions of 38, 50, and 79 microns, the whole having a Sauter mean diameter of 50 microns. Complete burnout was predicted for each of these sizes. When the particles are burned out they are no longer tracked. The carbon particles travel roughly half way across the chamber before they are consumed. Other cases were run with larger particle sizes. The maximum particle size for predicted complete carbon burnout was approximately 200 microns. This is smaller than the actual particle size in the carbon filters, which are millimeter sized particles (40% passing through U.S. mesh #12 (1.40 mm)). Therefore, a further grind would be required to ensure full burnout, which makes the LIC unattractive for carbon closure. This examples illustrates the utility of the model for evaluating strategies for handling contaminants such as the contaminants such as the carbon filters during decommissioning.

Metal Parts Furnace CFD Model

The three zone metal parts furnace is used for decontamination of relatively inert materials. Firing an auxiliary fuel with air provides high temperature combustion products. Metal parts pass intermittently through the furnace at a temperature of at least 540 °C and with a residence time of 15 minutes. During this time condensed agent decontamination is achieved through a combination of evaporation, decomposition and oxidation.

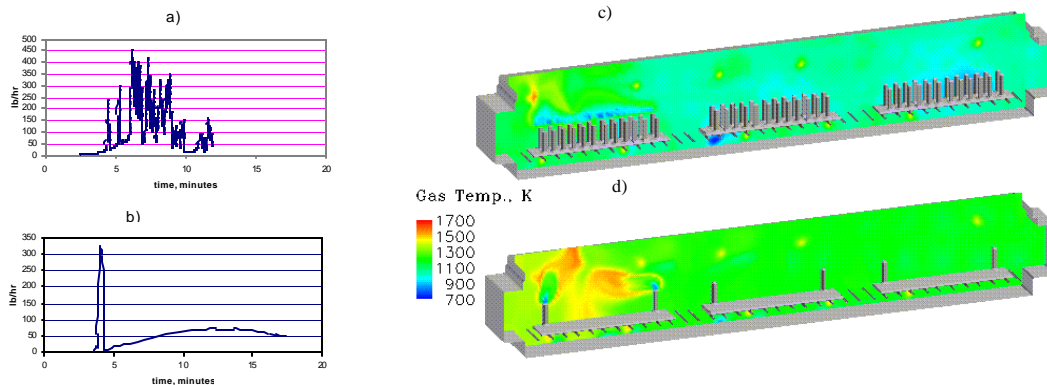


Figure 2 a) Total agent vaporization rate as a function of time for 48 155 mm projectiles with 5% residual agent.
 b) Total agent vaporization rate as a function of time for two full 155 mm projectiles.
 c) MPF primary chamber gas temperature with 48 projectiles with 5% residual agent.
 d) MPF primary chamber gas temperature with two full projectiles.

The MPF module consists of two parts: a transient projectile vaporization model and the combustion CFD model. A quasi-steady approach was used, as the CFD model is a steady state combustion model. This quasi-steady approach consisted of three steps:

1. The flow field and temperature fields were predicted with the CFD model using the heat sink of the feed and the expected maximum agent release rate.
2. A lumped two-node transient calculation of the projectile temperature and agent release rate was performed for each projectile on the tray using the heating rates predicted from the incident heat fluxes. These were obtained from the CFD solution.
3. The CFD solution was updated with the predicted agent release rate distribution and heat sinks at time of maximum agent release rate for the tray in zone 1. The agent release rate for the other two zones was zero. The temperature of the projectiles for the other two zones was taken from the projectile submodel prediction at the corresponding time for those zones.

A simple two-node projectile model was developed for the MPF model to predict the rate and distribution of agent release from 155mm projectiles containing GB simulant, DMMP. Nucleation boiling heat transfer between the projectile and liquid was included in the submodel. Figures 2a and 2b show the total agent release rate as a function of time for two tray configurations. The 48 projectile configuration was used for the baseline simulation. The heat flux to the first two trays is the highest because of the energy generated by the DMMP combustion. The projectiles in the interior of the tray receive less heat than those stacked on the sides. The interior projectiles are partially shielded from radiation from the furnace walls by the outer projectiles. Figure 2c shows the predicted gas temperature for the baseline case with 48 projectiles. The flame from the agent combustion can be seen above the front of the first tray where the majority of the agent is being released from the projectiles at this particular “snapshot” in time. Figure 2d shows the predicted gas temperature for a second case where two full projectiles are introduced into the furnace. Although the maximum release rate of the two full projectiles is less than the baseline (360 lb/hr versus 460 lb/hr), the gas temperatures above the projectiles are higher in the two full projectiles case. This is because only two projectiles are present on the tray providing a significantly smaller heat sink in the furnace. The same water quench rate was assumed in this prediction.

Detailed chemical kinetics calculations were performed along streamlines that originated at the tips of projectiles calculated to have large rates of agent release. The streamline kinetics calculations assume that the gas at the tip of the projectiles is 100% DMMP. Destruction takes place in the MPF within 0.1 seconds whereas residence times of these trajectories in the MPF approximately fall in the range 0.4-1.5 sec. It should be remembered that after the gases exit the MPF they are processed in the afterburner.

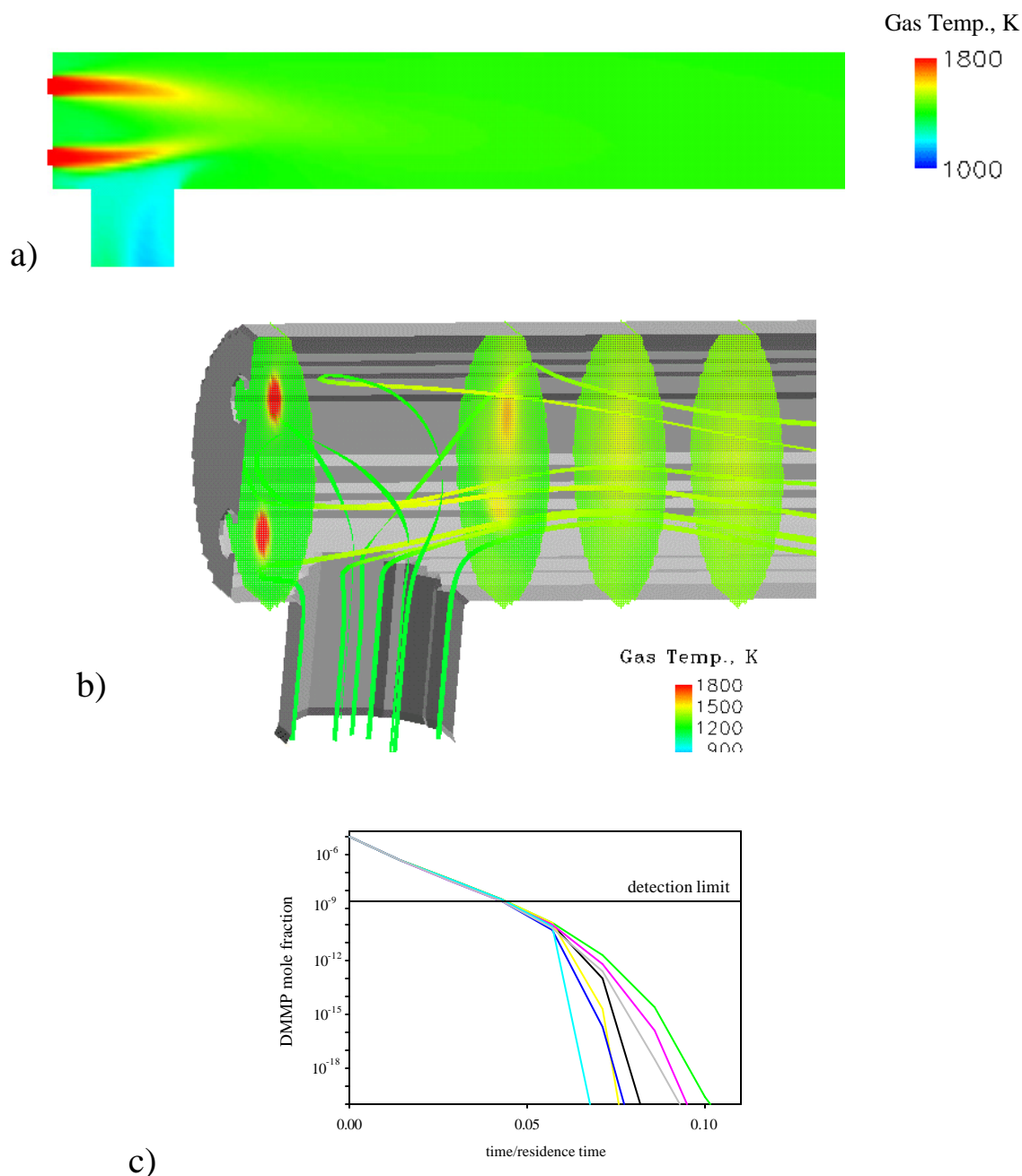


Figure 3 MPF Afterburner Simulation and DMMP destruction calculated along stream lines.

The MPF Afterburner CFD Model

In addition to providing a proof-of-concept for a typical afterburner, the MPF afterburner model provided a test bed for the application of detailed chemistry for agent destruction. A base case was created in which the velocity, temperature, and concentrations at the outlet of the MPF primary chamber CFD simulation discussed below were mapped to the inlet of the afterburner. Typical results are shown in Fig. 3 for the base case. The MPF afterburner includes two rapid mix, natural gas fired tunnel burners directed along the length of the afterburner chamber. The high temperature gases produced by these burners are shown in red in Figs. 3a and 3b. These figures show axial and

radial temperature profiles respectively. Also shown in Fig. 3b are representative streamlines entering the chamber. These are the mean paths of differential fluid elements calculated from the predicted flow field and they are colored by the local mean temperature. The tortuous path of some elements is because they are entrained in the backflow created by the afterburners. The streamline integrator described in the previous section was used with the full DMMP kinetic mechanism to calculate DMMP destruction. It was assumed that 5200 ppm of agent simulant DMMP enters the afterburner. This very high concentration assumes almost no destruction in the MPF primary chamber. As shown in Fig. 3c, the DMMP very rapidly breaks down to levels that are far below the detection limit. It should be noted that the calculated mean residence time in the afterburner is 1.4 seconds, which is far longer than needed to completely destroy the simulant.

We have integrated our 15-species reduced mechanism into our *GLACIER* postprocessor and run the two MPF afterburner cases (baseline and one burner out). In both cases the agent is destroyed in the duct connecting the furnace with the afterburner. The agent never reaches the auxiliary gas flames.

We have also run two upset conditions for the MPF afterburner. The first is a case with the lower burner disabled. The second upset condition makes the impossibly bad assumption that all of the agent released in the MPF enters the afterburner as a concentrated, unreacted “puff” of pure agent. To consider a worst-case scenario we have placed the puff to the side of the duct between the MPF and the afterburner to delay its interaction with the afterburner flames. Streamline calculations for these upset conditions show complete destruction of the agent within 0.25 seconds, whereas the residence time within the afterburner roughly 1.4 seconds.

Deactivation Furnace System CFD Model

The deactivation furnace System (DFS) is a gas-fired counterflow rotary kiln designed to treat energetics (fuses, boosters, bursters, and solid rocket propellant). Energetics are all contained in thin-walled metallic housings that must be punched or cut into pieces prior to burning; confined energetics would detonate in the kiln rather than burn.

The MPF module consists of two parts: an energetics/rocket piece combustion submodel and the gas phase combustion CFD model. A simple energetics combustion submodel was developed for the DFS kiln module, which consisted of tracking rocket pieces along the bottom of the kiln at a constant velocity corresponding to the rotational speed of the kiln (1.7 rpm) and the pitch of the spiral flights (30 inch pitch). The incident radiation field was used to calculate the rocket piece temperature and burn rate of the propellant as a function of time and axial position using an assumed propellant surface area. The source terms for the energetics and agent off-gas were calculated for use in the gas phase calculations. A propellant burn rate of 0.025 cm/s was estimated at the total pressure of the kiln. The most significant unknown in the energetics model is the propellant surface area of the sheared rocket pieces. The surface area of the propellant was assumed to be linearly proportional to the remaining propellant mass.

Figure 4 shows the predicted gas temperature and oxygen concentration in a vertical plane along the centerline-axis of the kiln. As seen in the figure, the propellant in the rocket pieces in this simulation started combusting at about one third the distance from the charge end of the kiln. The gas temperatures immediately around this region of maximum burn rate are about 2900 K. The oxygen is depleted around this region largely because of the equilibrium assumption used in this CFD calculation. The propellants contain their own oxidant so that the fuel and oxidant are already well mixed as energetics off-gas. Product species containing oxygen (CO_2 , CO , and H_2O , HOPO_2) are in higher concentration in this region of high temperature.

CONCLUSION

This paper has demonstrated that CFD models of key components of chemical demilitarization incinerators can be constructed and provide very useful information on the physical processes that affect their performance in terms of destruction efficiency and operability. Models have been demonstrated for the Liquid Incinerator (LIC), Metal Parts Furnace (MPF), MPF afterburner, and Deactivation Furnace System (DFS) kiln. The models have predicted complete destruction of the chemical agent when the incinerators and afterburners are operated as per standard operating conditions. The models may also be useful in simulating incineration system upset conditions and failures that could lead to an agent release, so that appropriate design and operational modifications can be made to mitigate such occurrences.

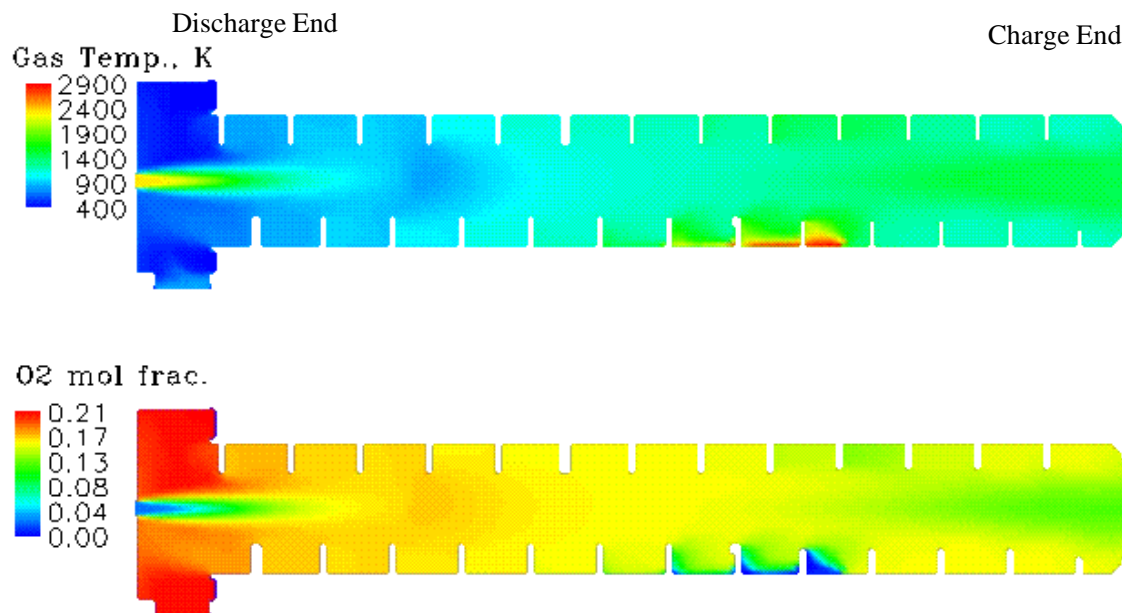


Figure 4 DFS - Gas Temperature and Oxygen Distributions.

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